



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:27 AM UTC

PDB ID : 1PG7 / pdb_00001pg7
Title : Murine 6A6 Fab in complex with humanized anti-Tissue Factor D3H44 Fab
Authors : Eigenbrot, C.; Meng, Y.G.; Krishnamurthy, R.; Lipari, M.T.; Presta, L.; Devaux, B.; Wong, T.; Moran, P.; Bullens, S.; Kirchhofer, D.
Deposited on : 2003-05-27
Resolution : 2.50 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

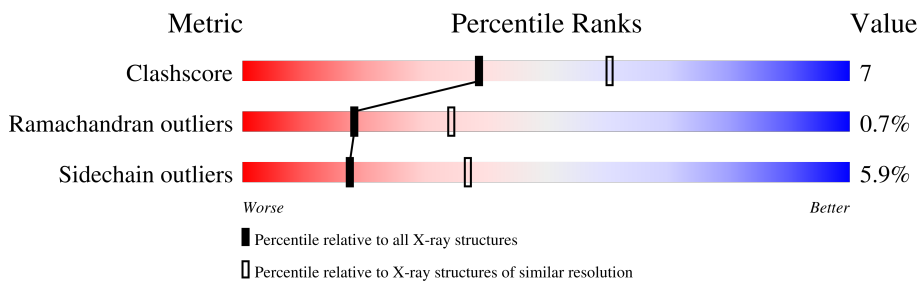
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	217	
1	I	217	
2	L	213	
2	M	213	
3	W	210	
3	Y	210	
4	X	220	
4	Z	220	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13317 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called humanized antibody D3H44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	213	Total 1600	C 1011	N 266	O 317	S 6	7	0	0
1	I	213	Total 1600	C 1011	N 266	O 317	S 6	3	0	0

- Molecule 2 is a protein called humanized antibody D3H44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	213	Total 1658	C 1038	N 280	O 335	S 5	11	1	0
2	M	213	Total 1647	C 1032	N 276	O 334	S 5	0	0	0

- Molecule 3 is a protein called murine antibody 6A6 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	W	210	Total 1581	C 988	N 265	O 323	S 5	5	0	0
3	Y	210	Total 1581	C 988	N 265	O 323	S 5	5	0	0

- Molecule 4 is a protein called murine antibody 6A6 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	X	220	Total 1688	C 1068	N 282	O 330	S 8	1	2	0
4	Z	220	Total 1688	C 1068	N 282	O 330	S 8	7	2	0

- Molecule 5 is water.

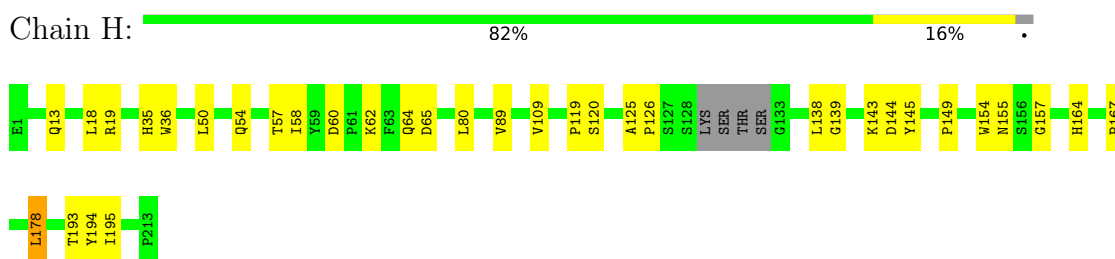
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	26	Total O 26 26	0	0
5	I	33	Total O 33 33	0	0
5	L	33	Total O 33 33	0	0
5	M	43	Total O 43 43	0	0
5	W	41	Total O 41 41	0	0
5	X	26	Total O 26 26	0	0
5	Y	38	Total O 38 38	0	0
5	Z	34	Total O 34 34	0	0

3 Residue-property plots [i](#)

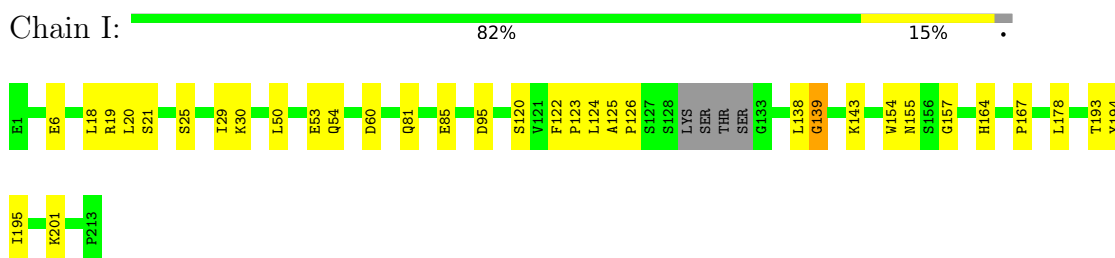
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

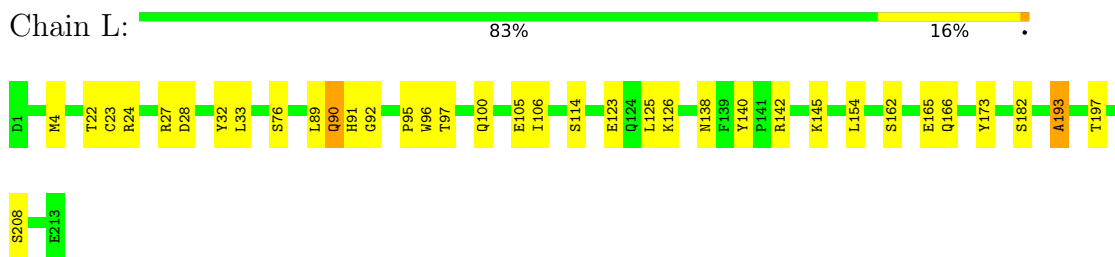
- Molecule 1: humanized antibody D3H44



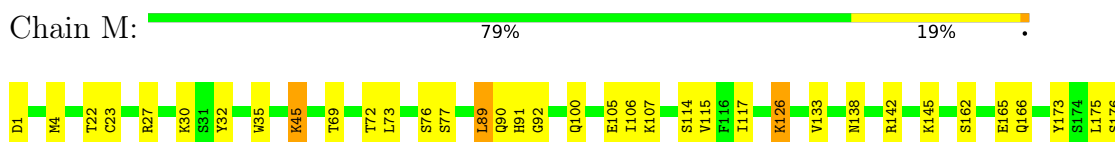
- Molecule 1: humanized antibody D3H44



- Molecule 2: humanized antibody D3H44

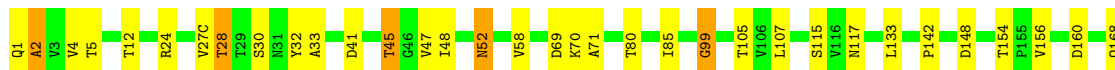
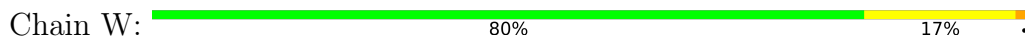


- Molecule 2: humanized antibody D3H44

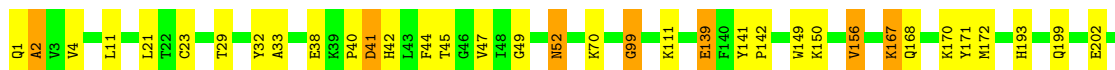
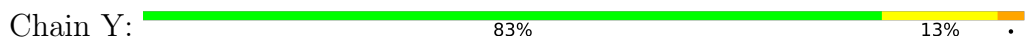




- Molecule 3: murine antibody 6A6 Fab fragment



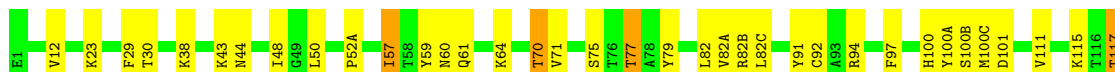
- Molecule 3: murine antibody 6A6 Fab fragment



- Molecule 4: murine antibody 6A6 Fab fragment



- Molecule 4: murine antibody 6A6 Fab fragment



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.89Å 85.78Å 92.37Å 77.48° 75.92° 63.33°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.9 (50.00-2.50)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.217 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13317	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H	0.54	0/1639	0.98	4/2236 (0.2%)
1	I	0.58	0/1639	0.98	6/2236 (0.3%)
2	L	0.56	0/1695	0.99	6/2301 (0.3%)
2	M	0.58	0/1684	0.98	8/2287 (0.3%)
3	W	0.57	0/1619	1.01	5/2211 (0.2%)
3	Y	0.57	0/1619	0.97	5/2211 (0.2%)
4	X	0.56	0/1733	1.01	10/2369 (0.4%)
4	Z	0.59	0/1733	0.99	5/2369 (0.2%)
All	All	0.57	0/13361	0.99	49/18220 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	101	ASP	N-CA-C	8.13	120.06	111.03
4	Z	143	LYS	N-CA-C	7.62	121.86	109.59
3	Y	47	VAL	CB-CA-C	-7.45	105.38	111.71
4	X	143	LYS	N-CA-C	7.25	121.27	109.59
2	L	76	SER	N-CA-C	7.07	120.02	111.82
1	I	143	LYS	N-CA-C	7.06	121.17	109.95
3	W	58	VAL	CA-C-N	6.97	127.01	119.90
3	W	58	VAL	C-N-CA	6.97	127.01	119.90
1	I	120	SER	N-CA-C	-6.85	98.07	109.24
4	X	60	ASN	N-CA-C	-6.79	98.97	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	106	ILE	N-CA-C	6.70	117.68	108.84
4	Z	120	SER	N-CA-C	-6.60	98.44	109.07
1	H	143	LYS	N-CA-C	6.59	120.43	109.95
4	Z	60	ASN	N-CA-C	-6.57	99.31	109.76
4	Z	101	ASP	N-CA-C	6.56	118.31	111.03
4	X	120	SER	N-CA-C	-6.38	98.84	109.24
2	M	193	ALA	N-CA-C	6.34	119.06	109.23
2	M	76	SER	N-CA-C	6.32	120.25	112.54
1	I	139	GLY	N-CA-C	6.29	119.67	110.80
1	H	120	SER	N-CA-C	-6.26	99.03	109.24
4	X	29	PHE	N-CA-C	6.08	118.69	111.33
2	L	193	ALA	N-CA-C	6.00	118.42	108.99
3	Y	170	LYS	N-CA-C	-6.00	102.07	110.35
2	L	114	SER	N-CA-C	-5.98	99.45	108.96
4	X	211	VAL	CA-C-N	5.94	125.88	119.76
4	X	211	VAL	C-N-CA	5.94	125.88	119.76
3	Y	202	GLU	N-CA-C	5.82	118.54	109.52
4	X	73	ARG	N-CA-C	5.76	118.50	111.82
3	W	180	THR	N-CA-C	-5.71	102.06	110.52
3	W	115	SER	N-CA-C	-5.70	99.89	108.96
2	M	114	SER	N-CA-C	-5.67	99.49	108.73
2	L	165	GLU	N-CA-C	-5.64	102.94	110.55
2	M	133	VAL	N-CA-C	5.63	116.06	108.17
1	I	124	LEU	N-CA-C	-5.62	97.03	107.71
1	H	89	VAL	N-CA-C	-5.52	99.78	108.23
3	W	99	GLY	N-CA-C	-5.52	104.16	112.89
2	M	165	GLU	N-CA-C	-5.51	103.11	110.55
2	M	106	ILE	N-CA-C	5.50	116.09	108.84
1	H	144	ASP	N-CA-C	5.30	118.43	111.28
2	L	182	SER	N-CA-C	-5.27	103.43	110.55
4	X	128	CYS	N-CA-C	-5.25	106.38	112.89
3	Y	139	GLU	N-CA-C	5.24	118.62	111.39
2	M	115	VAL	N-CA-C	5.24	116.51	108.71
4	Z	29	PHE	N-CA-C	5.12	119.81	111.37
1	I	60	ASP	N-CA-C	-5.11	101.98	109.50
4	X	100(B)	SER	N-CA-C	5.09	118.41	110.32
3	Y	99	GLY	N-CA-C	-5.08	104.86	112.89
1	I	125	ALA	N-CA-C	5.06	116.25	109.83
2	M	182	SER	N-CA-C	-5.00	103.80	110.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	140	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1600	0	1549	21	0
1	I	1600	0	1549	19	0
2	L	1658	0	1610	26	0
2	M	1647	0	1598	25	0
3	W	1581	0	1519	18	0
3	Y	1581	0	1519	21	0
4	X	1688	0	1650	25	0
4	Z	1688	0	1650	32	0
5	H	26	0	0	0	0
5	I	33	0	0	1	0
5	L	33	0	0	1	0
5	M	43	0	0	2	0
5	W	41	0	0	3	0
5	X	26	0	0	0	0
5	Y	38	0	0	1	0
5	Z	34	0	0	3	0
All	All	13317	0	12644	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:70:THR:HG23	4:X:79:TYR:HB2	1.50	0.91
3:Y:168:GLN:HG2	3:Y:172:MET:HE2	1.54	0.89
3:W:28:THR:HG23	3:W:30:SER:H	1.39	0.86
2:L:193:ALA:HB2	2:L:208:SER:HB3	1.60	0.83
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.23	0.74
2:M:166:GLN:HG3	2:M:173:TYR:CZ	2.24	0.73
4:X:70:THR:CG2	4:X:79:TYR:HB2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:139:GLU:HG2	3:Y:168:GLN:HE22	1.56	0.71
4:X:59:TYR:HE1	4:X:69:LEU:HD13	1.56	0.69
2:M:4:MET:HE3	2:M:23:CYS:SG	2.33	0.68
4:X:127:VAL:CG1	4:X:213:LYS:HD3	2.24	0.66
1:I:155:ASN:HD21	1:I:194:TYR:HA	1.61	0.66
4:Z:115:LYS:O	4:Z:117:THR:HG22	1.96	0.66
4:Z:61:GLN:HA	4:Z:64:LYS:HG3	1.77	0.65
2:L:100:GLN:HB2	5:L:234:HOH:O	1.97	0.64
4:X:123:PRO:HD3	4:X:208:LYS:HE2	1.80	0.64
4:Z:70:THR:HB	5:Z:638:HOH:O	1.97	0.63
4:Z:152:LEU:HD22	4:Z:197:VAL:HG22	1.80	0.63
3:W:85:ILE:CD1	4:X:43:LYS:HE3	2.29	0.62
1:H:126:PRO:HG3	1:H:138:LEU:HB3	1.82	0.62
4:X:100(A):TYR:N	4:X:100(A):TYR:CD1	2.68	0.61
4:X:18:VAL:HG12	4:X:82(C):LEU:HD11	1.82	0.61
4:X:100:HIS:CG	4:X:100:HIS:O	2.53	0.61
2:L:4:MET:CE	2:L:23:CYS:SG	2.89	0.61
2:M:32:TYR:HB3	2:M:91:HIS:CE1	2.36	0.60
1:H:155:ASN:HD21	1:H:194:TYR:HA	1.66	0.60
2:L:24[A]:ARG:HG3	2:L:24[A]:ARG:HH21	1.66	0.60
4:Z:100:HIS:O	4:Z:100:HIS:CG	2.55	0.60
4:Z:70:THR:HG22	4:Z:79:TYR:HB2	1.84	0.59
3:W:168:GLN:HB3	3:W:172:MET:HE2	1.84	0.59
1:I:126:PRO:HG3	1:I:138:LEU:HB3	1.85	0.59
2:M:145:LYS:HB3	2:M:197:THR:HB	1.85	0.59
3:W:24:ARG:NH1	3:W:70:LYS:HD3	2.18	0.59
2:M:27:ARG:HD2	3:Y:29:THR:HG23	1.85	0.58
3:W:5:THR:HG23	5:W:221:HOH:O	2.02	0.57
2:M:4:MET:HE2	2:M:90:GLN:HB2	1.87	0.56
4:Z:152:LEU:HG	4:Z:179:SER:CB	2.36	0.56
2:L:32:TYR:HD2	2:L:92:GLY:HA2	1.71	0.56
4:X:147:PRO:HD2	4:X:201:ALA:CB	2.37	0.55
1:H:139:GLY:HA2	1:H:154:TRP:CH2	2.42	0.55
4:X:119:PRO:HB3	4:X:145:TYR:HB3	1.89	0.55
1:H:36:TRP:CE2	1:H:80:LEU:HB2	2.41	0.55
1:I:18:LEU:HD12	1:I:18:LEU:O	2.07	0.55
3:W:28:THR:HG23	3:W:30:SER:N	2.18	0.55
1:H:35:HIS:HE1	2:L:96:TRP:CH2	2.24	0.54
2:L:4:MET:HE3	2:L:23:CYS:SG	2.47	0.54
4:Z:123:PRO:HD3	4:Z:208:LYS:HE2	1.89	0.54
1:I:18:LEU:O	1:I:19:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:THR:C	1:H:58:ILE:HD12	2.33	0.54
4:X:127:VAL:O	4:X:127:VAL:HG13	2.07	0.53
3:Y:111:LYS:HG2	5:Y:730:HOH:O	2.09	0.53
4:Z:100(A):TYR:CD1	4:Z:100(A):TYR:N	2.77	0.53
4:X:59:TYR:CE1	4:X:69:LEU:HD13	2.42	0.52
3:Y:23:CYS:O	3:Y:70:LYS:HB2	2.09	0.52
3:Y:168:GLN:HG2	3:Y:172:MET:CE	2.36	0.52
3:W:105:THR:HG21	3:W:142:PRO:HB3	1.91	0.52
2:M:27:ARG:HD2	3:Y:29:THR:CG2	2.40	0.51
4:X:115:LYS:O	4:X:117:THR:HG22	2.10	0.51
2:M:211:ARG:HG2	5:M:724:HOH:O	2.11	0.51
2:M:89:LEU:C	2:M:89:LEU:HD13	2.35	0.51
4:Z:23:LYS:NZ	4:Z:75:SER:O	2.42	0.51
2:M:185:ASP:O	2:M:188:LYS:HG2	2.10	0.51
1:H:18:LEU:HD23	1:H:109:VAL:HG11	1.93	0.51
2:L:193:ALA:CB	2:L:208:SER:HB3	2.36	0.51
3:W:4:VAL:O	3:W:99:GLY:HA2	2.11	0.51
4:Z:100:HIS:O	4:Z:100:HIS:ND1	2.44	0.51
2:M:100:GLN:H	2:M:100:GLN:CD	2.19	0.50
4:Z:127:VAL:HG11	4:Z:213:LYS:HE2	1.93	0.50
4:X:127:VAL:HG11	4:X:213:LYS:HD3	1.93	0.50
1:I:18:LEU:HD13	1:I:20:LEU:HG	1.95	0.49
1:I:155:ASN:ND2	1:I:195:ILE:H	2.09	0.49
4:Z:94:ARG:O	4:Z:100(C):MET:HA	2.13	0.49
3:W:45:THR:HB	5:W:234:HOH:O	2.13	0.49
1:H:18:LEU:CD2	1:H:109:VAL:HG11	2.43	0.49
1:H:58:ILE:HD12	1:H:58:ILE:N	2.28	0.49
2:M:32:TYR:HD2	2:M:92:GLY:HA2	1.77	0.48
4:X:166:PHE:HB3	4:X:167:PRO:HD2	1.95	0.48
4:Z:147:PRO:O	4:Z:199:HIS:HE1	1.97	0.48
2:L:32:TYR:HB3	2:L:91:HIS:CE1	2.48	0.48
3:Y:11:LEU:HD12	3:Y:21:LEU:CD2	2.44	0.48
2:L:4:MET:HE2	2:L:23:CYS:SG	2.52	0.48
1:I:164:HIS:HE1	2:M:138:ASN:OD1	1.97	0.48
3:W:148:ASP:O	3:W:193:HIS:HB2	2.14	0.48
1:H:60:ASP:HA	2:L:95:PRO:HB3	1.94	0.47
4:Z:57:ILE:HG13	4:Z:59:TYR:CE2	2.48	0.47
4:Z:184:THR:O	4:Z:187:THR:HB	2.13	0.47
4:Z:38:LYS:HB2	4:Z:48:ILE:HD11	1.95	0.47
1:H:50:LEU:C	1:H:50:LEU:HD12	2.38	0.47
4:X:50:LEU:HG	4:X:58:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:LEU:HD12	1:I:18:LEU:C	2.40	0.47
2:M:27:ARG:C	2:M:69:THR:HG22	2.40	0.47
2:L:27:ARG:NH1	2:L:28:ASP:O	2.48	0.47
1:H:155:ASN:ND2	1:H:195:ILE:H	2.12	0.46
3:W:173:ALA:HA	5:W:236:HOH:O	2.15	0.46
1:H:164:HIS:HE1	2:L:138:ASN:OD1	1.99	0.46
1:I:50:LEU:HD12	1:I:50:LEU:C	2.41	0.46
1:I:53:GLU:CD	4:Z:94:ARG:HH22	2.23	0.46
2:M:22:THR:HG22	2:M:23:CYS:N	2.31	0.46
2:M:89:LEU:HD13	2:M:90:GLN:N	2.31	0.46
1:I:139:GLY:HA2	1:I:154:TRP:CH2	2.52	0.45
3:Y:167:LYS:HD3	3:Y:171:TYR:CZ	2.52	0.45
4:X:127:VAL:HG12	4:X:213:LYS:HD3	1.97	0.45
1:H:167:PRO:HD2	2:L:162:SER:OG	2.17	0.45
2:L:90:GLN:NE2	2:L:97:THR:OG1	2.50	0.45
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.98	0.45
2:L:27:ARG:HH11	2:L:27:ARG:HG3	1.81	0.45
1:I:29:ILE:HD12	1:I:30:LYS:N	2.31	0.44
1:I:155:ASN:C	1:I:157:GLY:H	2.25	0.44
2:M:35:TRP:CE2	2:M:73:LEU:HB2	2.53	0.44
1:H:18:LEU:HD22	1:H:109:VAL:HG21	1.98	0.44
2:L:24[A]:ARG:HH21	2:L:24[A]:ARG:CG	2.29	0.44
4:X:154:TRP:CH2	4:X:195[B]:CYS:HB3	2.52	0.44
2:M:30:LYS:HB3	2:M:30:LYS:HE2	1.81	0.44
4:Z:12:VAL:O	4:Z:111:VAL:HA	2.18	0.44
3:Y:42:HIS:HB3	4:Z:91:TYR:OH	2.17	0.44
4:Z:50:LEU:C	4:Z:50:LEU:HD12	2.42	0.44
1:H:155:ASN:C	1:H:157:GLY:H	2.26	0.44
3:Y:141:TYR:HA	3:Y:142:PRO:C	2.43	0.44
2:L:126:LYS:HE2	2:L:126:LYS:HB3	1.89	0.44
4:X:177:LEU:C	4:X:177:LEU:HD23	2.43	0.43
3:Y:1:GLN:O	3:Y:2:ALA:HB3	2.18	0.43
4:X:50:LEU:C	4:X:50:LEU:HD12	2.44	0.43
2:M:100:GLN:HB2	5:M:662:HOH:O	2.19	0.43
3:Y:49:GLY:HA3	4:Z:100(B):SER:HB3	2.01	0.43
2:M:142:ARG:O	2:M:142:ARG:HD3	2.19	0.43
4:X:94:ARG:O	4:X:100(C):MET:HA	2.19	0.43
4:Z:162:GLY:O	4:Z:181:VAL:HA	2.19	0.43
1:H:35:HIS:HE1	2:L:96:TRP:CZ3	2.36	0.43
3:W:52:ASN:C	3:W:52:ASN:HD22	2.26	0.43
3:Y:32:TYR:O	3:Y:33:ALA:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:149:TRP:O	3:Y:156:VAL:HG13	2.19	0.43
1:I:53:GLU:OE2	4:Z:94:ARG:NH2	2.52	0.42
2:M:22:THR:CG2	2:M:23:CYS:N	2.82	0.42
3:W:1:GLN:O	3:W:2:ALA:HB3	2.19	0.42
3:W:203:LYS:HD3	3:W:203:LYS:HA	1.92	0.42
4:X:210:ILE:N	4:X:210:ILE:HD12	2.34	0.42
4:Z:170:LEU:HD13	4:Z:175:TYR:CE1	2.52	0.42
2:L:89:LEU:HD13	2:L:89:LEU:C	2.44	0.42
2:L:125:LEU:HD23	2:L:125:LEU:HA	1.78	0.42
3:W:27(C):VAL:HG11	3:W:71:ALA:HB2	2.01	0.42
4:Z:211:VAL:HB	4:Z:212:PRO:HD2	2.02	0.42
1:H:60:ASP:OD2	1:H:62:LYS:HD3	2.20	0.42
3:W:133:LEU:HB2	3:W:177:LEU:HB3	2.01	0.42
1:H:178:LEU:C	1:H:178:LEU:HD23	2.44	0.42
3:W:32:TYR:O	3:W:33:ALA:C	2.62	0.42
4:X:100(A):TYR:H	4:X:100(A):TYR:HD1	1.64	0.42
4:Z:30:THR:HA	4:Z:52(A):PRO:HB2	2.03	0.41
1:I:6:GLU:HA	1:I:21:SER:O	2.21	0.41
2:L:33:LEU:HD22	2:L:89:LEU:O	2.20	0.41
3:Y:38:GLU:HB2	3:Y:44:PHE:CE2	2.56	0.41
3:Y:52:ASN:HD22	3:Y:52:ASN:H	1.67	0.41
3:W:47:VAL:HG12	3:W:48:ILE:HG12	2.02	0.41
4:Z:212:PRO:HA	5:Z:683:HOH:O	2.20	0.41
1:H:125:ALA:HA	1:H:126:PRO:HD3	1.89	0.41
1:I:122:PHE:HA	1:I:123:PRO:HD3	1.90	0.41
2:L:193:ALA:HB2	2:L:208:SER:CB	2.43	0.41
4:X:29:PHE:CE2	4:X:52(A):PRO:HB3	2.56	0.41
3:Y:52:ASN:HD22	3:Y:52:ASN:N	2.19	0.41
4:Z:71:VAL:HG12	5:Z:737:HOH:O	2.21	0.41
4:Z:119:PRO:HB3	4:Z:145:TYR:HB3	2.02	0.41
1:I:126:PRO:HA	5:I:239:HOH:O	2.19	0.41
2:L:166:GLN:HG3	2:L:173:TYR:CE1	2.55	0.41
2:M:45:LYS:HB3	2:M:45:LYS:HE2	1.71	0.41
2:L:145:LYS:HB3	2:L:197:THR:HB	2.04	0.40
4:Z:127:VAL:HB	4:Z:213:LYS:HG3	2.04	0.40
1:I:167:PRO:HD2	2:M:162:SER:OG	2.21	0.40
2:M:126:LYS:HE3	2:M:126:LYS:HB2	1.88	0.40
2:M:175:LEU:HD23	2:M:176:SER:N	2.37	0.40
4:Z:23:LYS:HD2	4:Z:77:THR:HG22	2.03	0.40
3:Y:4:VAL:O	3:Y:99:GLY:HA2	2.21	0.40
3:Y:150:LYS:HD3	3:Y:193:HIS:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:ASP:OD1	1:I:95:ASP:C	2.64	0.40
3:Y:40:PRO:O	3:Y:41:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	209/217 (96%)	199 (95%)	9 (4%)	1 (0%)	24	43
1	I	209/217 (96%)	199 (95%)	10 (5%)	0	100	100
2	L	212/213 (100%)	207 (98%)	5 (2%)	0	100	100
2	M	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
3	W	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	12	24
3	Y	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	12	24
4	X	220/220 (100%)	204 (93%)	13 (6%)	3 (1%)	9	17
4	Z	220/220 (100%)	205 (93%)	12 (6%)	3 (1%)	9	17
All	All	1697/1720 (99%)	1612 (95%)	74 (4%)	11 (1%)	18	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	44	ASN
4	X	127	VAL
4	Z	127	VAL
3	Y	41	ASP
4	Z	44	ASN
1	H	64	GLN
3	W	41	ASP
3	W	2	ALA

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Mol	Chain	Res	Type
3	Y	2	ALA
4	X	149	PRO
4	Z	149	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	176/180 (98%)	169 (96%)	7 (4%)	28	54
1	I	176/180 (98%)	169 (96%)	7 (4%)	28	54
2	L	188/187 (100%)	182 (97%)	6 (3%)	34	62
2	M	187/187 (100%)	176 (94%)	11 (6%)	18	37
3	W	176/176 (100%)	164 (93%)	12 (7%)	14	31
3	Y	176/176 (100%)	171 (97%)	5 (3%)	38	66
4	X	195/193 (101%)	172 (88%)	23 (12%)	5	11
4	Z	195/193 (101%)	179 (92%)	16 (8%)	10	23
All	All	1469/1472 (100%)	1382 (94%)	87 (6%)	18	37

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	13	GLN
1	H	19	ARG
1	H	54	GLN
1	H	65	ASP
1	H	149	PRO
1	H	178	LEU
1	H	193	THR
1	I	25	SER
1	I	54	GLN
1	I	81	GLN
1	I	85	GLU
1	I	178	LEU

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Mol	Chain	Res	Type
1	I	193	THR
1	I	201	LYS
2	L	22	THR
2	L	90	GLN
2	L	105	GLU
2	L	123	GLU
2	L	142	ARG
2	L	154	LEU
2	M	1	ASP
2	M	45	LYS
2	M	72	THR
2	M	77	SER
2	M	89	LEU
2	M	105	GLU
2	M	107	LYS
2	M	117	ILE
2	M	126	LYS
2	M	190	LYS
2	M	204	PRO
3	W	12	THR
3	W	28	THR
3	W	45	THR
3	W	52	ASN
3	W	69	ASP
3	W	80	THR
3	W	107	LEU
3	W	117	ASN
3	W	154	THR
3	W	156	VAL
3	W	160	ASP
3	W	205	LEU
4	X	1	GLU
4	X	5	GLN
4	X	13	LYS
4	X	17	SER
4	X	54	ASN
4	X	57	ILE
4	X	62	LYS
4	X	71	VAL
4	X	82	LEU
4	X	82(A)	VAL
4	X	82(B)	ARG

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Mol	Chain	Res	Type
4	X	82(C)	LEU
4	X	97	PHE
4	X	105	GLN
4	X	117	THR
4	X	138	LEU
4	X	149	PRO
4	X	152	LEU
4	X	177	LEU
4	X	181	VAL
4	X	186	SER
4	X	195[A]	CYS
4	X	195[B]	CYS
3	Y	45	THR
3	Y	52	ASN
3	Y	156	VAL
3	Y	167	LYS
3	Y	199	GLN
4	Z	43	LYS
4	Z	57	ILE
4	Z	70	THR
4	Z	77	THR
4	Z	82	LEU
4	Z	82(A)	VAL
4	Z	82(B)	ARG
4	Z	82(C)	LEU
4	Z	92	CYS
4	Z	97	PHE
4	Z	117	THR
4	Z	128	CYS
4	Z	131	THR
4	Z	138	LEU
4	Z	152	LEU
4	Z	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	13	GLN
1	H	73	ASN
1	H	155	ASN
1	H	164	HIS
1	H	192	GLN

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Mol	Chain	Res	Type
1	I	39	GLN
1	I	64	GLN
1	I	82(A)	ASN
1	I	155	ASN
1	I	164	HIS
2	L	3	GLN
2	L	160	GLN
2	L	199	GLN
2	L	210	ASN
2	M	37	GLN
2	M	38	GLN
3	W	34	ASN
3	W	52	ASN
3	W	117	ASN
3	W	169	ASN
3	W	196	HIS
4	X	39	GLN
4	X	171	GLN
3	Y	52	ASN
3	Y	79	GLN
3	Y	117	ASN
3	Y	164	GLN
3	Y	168(B)	ASN
3	Y	193	HIS
3	Y	199	GLN
4	Z	5	GLN
4	Z	41	HIS
4	Z	199	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.